The Quantum Information Police: Making Pairing Wave Functions Behave Themselves Using Correlator Product States

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Pairing wave functions, in which a two-particle object replaces a one particle orbital as the fundamental building block, have long been investigated as an alternative to mean field theory for addressing difficult problems in the electronic structure of molecules and materials. However, the various types of pairing approximations each possess severe shortcomings, such as the inability of perfect pairing to deal with multiple resonance structures and the antisymmetric geminal power's severe size consistency problem. We have recently shown that the latter problem can be eliminated by introducing a correlator product state, a wave function ansatz originally developed in the context of quantum information theory for use in low entanglement systems. We will present the key ideas behind this combination along with a collection of promising preliminary results in such difficult systems as the Hubbard model and chemical bond dissociations.